Quantal Overlapping Resonance Criterion: the Pullen Edmonds Model [1]

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Abstract

In order to highlight the onset of chaos in the Pullen-Edmonds model a quantal analog of the resonance overlap criterion has been examined. A quite good agreement between analytical and numerical results is obtained.

Recently great interest has been shown in the so–called *quantum chaos*, or more precisely *quantum chaology*, i.e. the study of quantal systems which are chaotic in the classical limit $\hbar \to 0$ [1].

The aim of this work is to apply a quantal analog of the resonance criterion [2] to the Pullen Edmonds model [3], in order to highlight the onset of chaos in a schematic model. A requisite for the occurrence of quantum chaos is that the spectrum behaves in an irregular way as a function of the coupling constant: in particular if multiple avoided crossings occur (see for example [4] and references quoted therein). In fact, as stressed by Berry [5], in *quasi–integrable systems* the presence of many quasi–crossings leads to a chaotic behaviour. Using the semiclassical quantization we calculate the critical value χ_c of the coupling constant corresponding to the intersection of two neighboring quantal separatrices. This criterion is, in some sense, the quantal counterpart of the method of overlapping resonances developed by Chirikov [6]. We point out however that the Pullen Edmonds hamiltonian is the perturbation of an intrinsically resonant hamiltonian (see e.g.[7] and references quoted therein) which yields intrinsically degenerate quantum unperturbed levels: hence we first have have to extend to this situation the argument of [2], valid in the case of accidental degenaracy.

As discussed by Pullen and Edmonds [4], the hamiltonian:

$$H = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + \chi q_1^2 q_2^2, \tag{1}$$

exhibits a transition from order to chaos as a function of the coupling constant

χ. We introduce the new variables (I, θ) by the canonical transformation:

$$\left\{ \begin{array}{lcl} q_i & = & \sqrt{2I_i}\cos\theta_i \\ p_i & = & \sqrt{2I_i}\sin\theta_i. \end{array} \right. \qquad i = 1, 2. \tag{2}$$

Then (1) becomes:

$$H = I_1 + I_2 + 4\chi I_1 I_2 \cos^2\theta_1 \cos^2\theta_2. \tag{3}$$

By the new canonical transformation:

$$\left\{ \begin{array}{lcl} A_1 & = & I_1 + I_2 \\ A_2 & = & I_1 - I_2 \end{array} \right. \qquad \left\{ \begin{array}{lcl} \theta_1 & = & \phi_1 + \phi_2 \\ \theta_2 & = & \phi_1 - \phi_2, \end{array} \right. \tag{4}$$

H can be written:

$$H = A_1 + \chi(A_1^2 - A_2^2)\cos^2(\phi_1 + \phi_2)\cos^2(\phi_1 - \phi_2). \tag{5}$$

We now eliminate the dependence on the angles to order χ^2 by resonant (or secular) canonical perturbation theory [8]. First we average on the fast variable (ϕ_1). This yields:

$$\frac{1}{2\pi}\int_0^{2\pi} d\phi_1 \cos^2(\phi_1 + \phi_2)\cos^2(\phi_1 - \phi_2) = \frac{1}{8}(2 + \cos 4\phi_2), \tag{6}$$

and:

$$\bar{H}_{cl} = A_1 + \frac{\chi}{8}(A_1^2 - A_2^2)(2 + \cos 4\phi_2). \tag{7}$$

The dependence on ϕ_2 is now eliminated by a second canonical transformation. The Hamilton–Jacobi equation for the perturbation part is indeed:

$$[A_1^2 - (\frac{\partial S}{\partial \phi_2})^2](2 + \cos 4\phi_2) = K, \tag{8}$$

$$\frac{\partial S}{\partial \phi_2} = \pm\sqrt{\frac{A_1^2(2 + \cos 4\phi_2) - K}{2 + \cos 4\phi_2}}. \tag{9}$$

and thus the Hamiltonian (7) becomes:

$$\bar{H} = B_1 + \frac{\chi}{8} K(B_1, B_2), \tag{10}$$

where:

$$B_1 = A_1, \quad B_2 = \frac{1}{2\pi} \oint d\phi_2 \frac{\partial S}{\partial \phi_2}. \tag{11}$$

It appears from the structure of equation (8) that the motion of our system is similar that of a simple pendulum:

$$\begin{array}{cc} 0 < K < B_1^2 & \textit{rotational motion} \\ K = B_1^2 & \textit{separatrix} \\ B_1^2 < K < 3B_1^2 & \textit{librational motion.} \end{array} \tag{12}$$

On the separatrix:

$$B_1^2(2 + \cos 4\phi_2) = K, \tag{13}$$

and:

$$B_2 = \pm \frac{2}{\pi} \int_a^b dx \sqrt{\frac{B_1^2(2 + \cos 4x) - K}{2 + \cos 4x}}, \tag{14}$$

where:

$$\begin{array}{cc} a = -\frac{\pi}{4}, \;\; b = \frac{\pi}{4} & \textit{rotational motion} \\ a = \phi_-(K, B_1), \;\; b = \phi_+(K, B_1) & \textit{librational motion} \end{array} \tag{15}$$

with:

$$\phi_\pm(K, B_1) = \pm \frac{1}{4} \arccos(\frac{K}{B_1^2} - 2). \tag{16}$$

The semiclassical quantization on the Hamiltonian (10) may be used. Set:

$$B_1 = m_1 \hbar, \;\; B_2 = m_2 \hbar; \tag{17}$$

then [9], up to terms of order $\hbar$, the quantum spectrum is:

$$E_{m_1,m_2} = m_1\hbar + \frac{\chi}{8}K(m_1\hbar, m_2\hbar), \tag{18}$$

where K is implicitly defined by the relation:

$$m_2\hbar = \pm\frac{2}{\pi}\int_a^b dx\sqrt{\frac{(m_1\hbar)^2(2+\cos 4x) - K}{2+\cos 4x}}, \tag{19}$$

and:

$$\begin{array}{cc} a = -\frac{\pi}{4}, \;\; b = \frac{\pi}{4} & 0 < K < (m_1\hbar)^2 \\ a = \phi_-(K, B_1), \;\; b = \phi_+(K, B_1) & (m_1\hbar)^2 < K < 3(m_1\hbar)^2 \end{array} \tag{20}$$

On the separatrix, where $K = (m_1\hbar)^2$, $m_2 = \pm\alpha m_1$, with:

$$\alpha = \frac{2}{\pi}\int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} dx\sqrt{\frac{1+\cos 4x}{2+\cos 4x}}. \tag{21}$$

Figure 1 shows K *vs* m_2.

By (18) it is not difficult to calculate the critical value χ_c of the coupling constant corresponding to the intersection of the separatrices of two neighboring multiplets:

$$(m_1+1)\hbar + \frac{\chi}{8}K[(m_1+1)\hbar, \alpha(m_1+1)\hbar] = m_1\hbar + \frac{\chi}{8}K(m_1\hbar, \alpha m_1\hbar), \tag{22}$$

and so:

$$\chi_c = \frac{-8\hbar}{K[(m_1+1)\hbar, \alpha(m_1+1)\hbar] - K(m_1\hbar, \alpha m_1\hbar)}. \tag{23}$$

The denominator of (23) can be evaluated by the Taylor expansion and finally:

$$\chi_c = \left[\frac{-8}{\frac{\partial K}{\partial B_1} - \alpha\frac{\partial K}{\partial B_2}}\right]_{B_1 = m_1\hbar, B_2 = \alpha m_2\hbar}. \tag{24}$$

K is implicitly defined by the relation:

$$F[B_1, B_2, K(B_1, B_2)] = B_2 - \frac{\pi}{2} \int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} dx \sqrt{\frac{B_1^2(2+\cos 4x) - K}{2+\cos 4x}} = 0, \qquad (25)$$

or:

$$F(B_1, B_2, K) = B_2 - \Phi(B_1, K) = 0. \qquad (26)$$

As a function of Φ, χ_c can be written:

$$\chi_c = \lim_{K \to B_1^2} \left[\frac{8 \frac{\partial \Phi}{\partial K}}{\alpha - \frac{\partial \Phi}{\partial B_1}} \right]_{B_1 = m_1 \hbar}, \qquad (27)$$

where:

$$\frac{\partial \Phi}{\partial K} = -\frac{1}{\pi} \int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} dx \frac{1}{\sqrt{(2+\cos 4x)[B_1^2(2+\cos 4x) - K]}}$$

$$\frac{\partial \Phi}{\partial B_1} = \frac{2}{\pi} \int_{-\frac{\pi}{4}}^{\frac{\pi}{4}} dx \sqrt{\frac{B_1^2(2+\cos 4x)}{B_1^2(2+\cos 4x) - K}}. \qquad (28)$$

It is not difficult to show that:

$$\chi_c = \frac{4}{m_1 \hbar}. \qquad (29)$$

Figure 2 shows χ_c *vs* $m_1\hbar$. If we take the energy $E \simeq m_1\hbar$ we obtain $\chi_c \simeq 4/E$, a quantal rule for the onset of classical chaos.

The transition order–chaos in systems with two degrees of freedom may be also studied by the curvature criterion of potential energy [10,11]. It is however important to point out that *in general* the curvature criterion guarantees only a *local instability* and should therefore be combined with the Poincarè sections [14]. For a fuller discussion of this point see [12].

At low energy, the motion near the minimum of the potential $V(q_1,q_2) = \frac{1}{2}(q_1^2+q_2^2)+\chi q_1^2 q_2^2$, where the curvature is positive, is periodic or quasiperiodic and is separated from the region of instability by a line of zero curvature; if the energy is increased, the system will be for some initial conditions in a region of negative curvature, where the motion is chaotic. In accordance with this scenario, the energy of order$\rightarrow$chaos transition E_c is equal to the minimum value of the line of zero gaussian curvature $K(q_1,q_2)$ of the potential–energy surface of the system. For our potential the gaussian curvature vanishes at the points that satisfy the equation:

$$\frac{\partial^2 V}{\partial q_1^2}\frac{\partial^2 V}{\partial q_2^2}-(\frac{\partial^2 V}{\partial q_1 \partial q_2})^2 = (2\chi q_1^2+1)(2\chi q_2^2+1)-16\chi^2 q_1^2 q_2^2 = 0. \tag{30}$$

It is easy to show that the minimal energy on the zero–curvature line is given by [13]:

$$E_c = V_{min}(K=0,\bar{r_1}) = \frac{4}{3\chi}, \tag{31}$$

and occurs at $\bar{q_1} = \pm\sqrt{\frac{1}{2\chi}}$. This result is in rough agreement with equation (29) and with the numerical calculations of Poincarè sections [14] obtained by authors of reference [3]. The discrepancy between (29) and (31) is due to the fact that the curvature criterion describes the onset of *local chaos* associated to quasi–crossings between levels of the same multiplet (see also reference [3]) meanwhile the quantum resonance criterion describes the onset of *widespread chaos* associated to quasi–crossings between separatices of different multiplets.

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Figure Captions

Figure 1: The semiclassical energy K *vs* m_2 for a fixed m_1: $0 < K < 1$ rotational motion (a) and $1 < K < 3$ librational motion (b).

Figure 2: The critical value χ_c *vs* $m_1\hbar$.

References

[1] A.M. Ozorio de Almeida: *Hamiltonian Systems: Chaos and Quantization*, Cambridge University Press (1990); M.C. Gutzwiller: *Chaos in Classical and Quantum Mechanics*, Berlin, Heidelberg, New York: Springer Verlag (1990); *From Classical to Quantum Chaos*, Conference Proceedings SIF, vol 41, Ed. G.F. Dell'Antonio, S. Fantoni, V.R. Manfredi (Editrice Compositori, Bologna, 1993).

[2] S. Graffi, T. Paul, H.J. Silverstone: Phys. Rev. Lett. **59**, 255 (1987); S. Graffi, T. Paul, H.J. Silverstone: Phys. Rev. A **37**, 2214 (1988)

[3] R.A. Pullen, R.A. Edmonds: J. Phys. A **14**, L477 (1981)

[4] V.R. Manfredi, L. Salasnich, L. Demattè: *Phys. Rev.* E **47**, 4556 (1993)

[5] M.V. Berry: in *Chaootic Behaviour in Quantum Systems*, Nato Series B, vol. 120, Ed. G. Casati (1983)

[6] B.V. Chirikov: *Phys. Rep.* **52**, 263 (1979)

[7] S. Graffi: in *Probabilistic Methods in Mathematical Physics*, Ed. F. Guerra, M.I. Loffredo, C. Marchioro (World Scientific, New York, 1991)

[8] M. Born: *Mechanics of the Atom* (Bell, London, 1960); T. Uzer, D.W. Noid, R.A. Marcus: *J. Chem. Phys.* **79**, 4412 (1983)

[9] S. Graffi, V.R. Manfredi, L. Salasnich: Preprint DFPD/TH/93, to be published.

[10] M. Toda: *Phys. Lett.* A **48**, 335 (1974)

[11] Yu. Bolotin, V.Yu. Gonchar, E.V. Inopin, V.V. Levenko, V.N. Tarasov, N.A. Chekanov: *Sov. I. Part. Nucl.* **20**, 372 (1989)

[12] G. Benettin, R. Brambilla, L. Galgani: *Physica* A **87**, 381 (1977)

[13] W.H. Steeb, A. Kunick: *Lett. Nuovo Cimento* **42**, 89 (1985)

[14] H. Poincarè: *New Methods of Celestial Mechanics*, vol. 3, ch. 27 (Transl. NASA Washington DC 1967); M. Henon: *Physica* D **5**, 412 (1982)